

Enhancing the spectral gap of networks by node removal

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Abstract

Dynamics on networks are often characterized by the second smallest eigenvalue of the Laplacian matrix of the network, which is called the spectral gap. Examples include the threshold coupling strength for synchronization and the relaxation time of a random walk. A large spectral gap is usually associated with high network performance, such as facilitated synchronization and rapid convergence. In this study, we seek to enhance the spectral gap of undirected and unweighted networks by removing nodes because, practically, the removal of nodes often costs less than the addition of nodes, addition of links, and rewiring of links. In particular, we develop a perturbative method to achieve this goal. The proposed method realizes better performance than other heuristic methods on various model and real networks. The spectral gap increases as we remove up to half the nodes in most of these networks.

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I. INTRODUCTION

Various systems of interacting elements can be represented by networks that consist of a set of nodes and links that connect pairs of nodes. The structure of networks affects various dynamics occurring on the networks [1–3]. In particular, many dynamics on networks are controlled by a few extremal eigenvalues of the adjacency matrix and the Laplacian matrix of the network (see Sec. II for the definition of the Laplacian matrix). The values of these eigenvalues provide concise and useful information about the dynamics on the networks.

In this study, we focus on the second smallest eigenvalue of the Laplacian matrix; it is called the spectral gap and is denoted by λ_2 in this paper. We examine λ_2 because it characterizes a wide class of dynamics on networks as follows. First, a network with a large value of λ_2 decreases the threshold of coupling strength for synchronization for both linear dynamics and some nonlinear dynamics including coupled oscillators on networks [1–6, 8]. Such a family of nonlinear dynamics is called the class II [2, 9] or type II [4] dynamics. Note that the largest Laplacian eigenvalue as well as λ_2 is an important determinant of the synchronizability in the so-called class III [2, 9] or type I [4] dynamics. However, we are not concerned with class III or type I dynamics in this paper. Second, when λ_2 is large, synchronization in these dynamics [5] and consensus dynamics [10] occur rapidly in certain types of networks. Third, λ_2 characterizes the convergence speed of the Markov chain on the network to the stationary density [8, 11]. Fourth, the first-passage time of the random walk is characterized by λ_2 [8]. Fifth, the duality between the coalescing random walk and the voter model [12] implies that λ_2 also determines the consensus time of the stochastic voter dynamics. This is in agreement with the results obtained for the majority-vote spin dynamics on networks [5]. In addition to these dynamical properties of networks, various graph-theoretical structural properties of networks are characterized by λ_2 [11, 13].

In these applications, a large value of λ_2 is usually preferred because it indicates, for example, enhanced synchronizability and fast convergence. Consequently, the enhancement of λ_2 has been explored in the framework of designing of networks [6, 7] and numerical optimization via the rewiring of links [8, 14]. In practice, however, rewiring links, constructing optimized networks from scratch, and adding nodes or links are likely to cost more than the removal of nodes or links of a given network. The effects of removal of nodes or links have been investigated in the context of the cascading failure [15] and the influence on extreme eigenvalues

of the adjacency matrix [16]. With regard to Laplacian eigenvalues, the removal of links always decreases λ_2 and makes the network less likely to synchronize [17, 18]. However, to the best of our knowledge, whether or not careful removal of nodes may increase λ_2 has not yet been examined. We treat this problem in the present paper.

Although removal of nodes generally decreases the magnitude of activities, stabilizing synchronization at the expense of the magnitude is valuable in some applications. The treatment of cardiac arrhythmia is one of the examples. The heart consists of a large number of cardiac cells that show nonlinear dynamics [19]. Synchronized dynamics of cardiac cells create physiological heart beats [20]. Cardiac arrhythmia is considered to be caused by malfunction of synchronization. The catheter ablation aims at restoring synchrony of the entire heart by electrically deactivating some cardiac cells that prevent synchronization [21]. As another example, proper operations of power plant networks also critically require that the frequency of voltage among power plants is synchronized [22, 23]. Loss of the synchronization may induce a blackout in the entire network. Therefore, it is likely that stable synchrony at the expense of some total power supply serves steady supplying of electricity to the entire network [22].

We compare various strategies for maximizing λ_2 by sequential node removal on various model and real networks. In particular, we develop a perturbative strategy that is applicable to relatively large networks in terms of the computational cost. We show that the performance of the perturbative strategy is comparable to that of the computationally costly optimal sequential strategy and is generally better than that of heuristic strategies. In addition, in many examined examples, λ_2 continues to increase until we remove a fairly large fraction of nodes ($\approx 50\%$) sequentially according to the perturbative strategy.

II. STRATEGIES FOR SEQUENTIAL NODE REMOVAL

We consider undirected and unweighted connected networks with N nodes. The Laplacian matrix L is defined as follows. L_{ij} ($1 \leq i \neq j \leq N$) is equal to -1 if node i and j are connected and 0 otherwise; L is a symmetric matrix. The diagonal is given by $L_{ii} = k_i$, where k_i is the degree of node i . Note that $\sum_{j=1}^N L_{ij} = 0$ for each i . L has N (real) nonnegative eigenvalues $0 = \lambda_1 < \lambda_2 \leq \dots \leq \lambda_N$. We seek to maximize λ_2 upon sequential removal of nodes. We compare the effectiveness of the following node removal strategies by applying them to model and real networks.

- *Degree-based strategy*: In each step, we remove the node with the smallest degree in the remaining network. The rationale behind this strategy is that the smallest degree controls λ_2 , with a useful bound being $\lambda_2 \leq k_{\min}N/(N-1)$, where k_{\min} is the smallest degree in the network [4, 11, 13]. If there exist multiple nodes having the same smallest degree, we select one of them with an equal probability.

In intentional attacks on networks, where the aim is to fragment the network into disjoint components with a small number of removed nodes, removing nodes with the largest degree is an effective strategy [24]. We implemented this strategy but obtained poor results for our purpose, and therefore we do not mention it in the following.

- *Betweenness-based strategy*: In each step, we remove the node with the smallest betweenness centrality. The betweenness centrality of node i is defined as follows. Denote by $\sigma_{i_1 i_2}$ the number of the shortest paths between nodes i_1 and i_2 , and by $\sigma_{i_1 i_2}(i)$ the number of the shortest paths between them that pass through node i . We set $\sigma_{i_1 i_2}(i_1) = \sigma_{i_1 i_2}(i_2) = 0$. The betweenness centrality of node i is proportional to $\sum_{i_1=1; i_1 \neq i}^N \sum_{i_2=i_1+1; i_2 \neq i}^N \sigma_{i_1 i_2}(i)/\sigma_{i_1 i_2}$ [2, 3, 25]. Sequentially removing nodes with the largest betweenness centrality yielded poor results, and therefore we do not mention it in the following.
- *Optimal sequential strategy*: We calculate the change in λ_2 induced by the removal of each node by direct numerical simulations. Then, we select the node whose removal increases λ_2 by the largest amount. Note that this strategy is computationally costly because it requires the calculation of λ_2 for N different networks, each having $N-1$ nodes. Calculating λ_2 for a single network requires $O(N^3)$ time. Therefore, carrying out a single step of the optimal sequential strategy requires $O(N^4)$ time.
- *Perturbative strategy*: To avoid the computational cost of the optimal sequential strategy, we develop an approximate perturbative strategy defined as follows. Related perturbative calculations are treated in [16, 17, 26].

Let us represent the eigen equation for λ_2 as $L\mathbf{u} = \lambda_2\mathbf{u}$, where \mathbf{u} is the N -dimensional eigenvector of L corresponding to λ_2 . The eigenvector \mathbf{u} is normalized such that $\sum_{i=1}^N u_i^2 = 1$, where u_i is the i th element of \mathbf{u} . The eigen equation after the removal

of node i is given by

$$(L + \Delta L)(\mathbf{u} + \Delta \mathbf{u}) = (\lambda_2 + \Delta \lambda_2)(\mathbf{u} + \Delta \mathbf{u}), \quad (1)$$

where the changes in L , λ_2 , and \mathbf{u} induced by the removal of node i are denoted by ΔL , $\Delta \lambda_2$, and $\Delta \mathbf{u}$, respectively. Because L is symmetric, the displacement matrix ΔL is given by $(\Delta L)_{ii} = -L_{ii} = -k_i$, $(\Delta L)_{jj} = L_{jj} (j \neq i)$, and $(\Delta L)_{ji} = (\Delta L)_{ij} = -L_{ji} (j \neq i)$. Because the i th component of $\mathbf{u} + \Delta \mathbf{u}$ is equal to zero, we write $\Delta \mathbf{u} = \delta \mathbf{u} - u_i \hat{\mathbf{e}}_i$, where $\hat{\mathbf{e}}_i$ is the unit vector for the i th component and $\delta \mathbf{u}$ is an N -dimensional vector. By multiplying the normalized left eigenvalue \mathbf{u}^\top (\top denotes the transpose) from the left of Eq. (1), we obtain

$$\Delta \lambda_2 = \frac{\mathbf{u}^\top \Delta L (\mathbf{u} - u_i \hat{\mathbf{e}}_i + \delta \mathbf{u})}{\mathbf{u}^\top (\mathbf{u} - u_i \hat{\mathbf{e}}_i + \delta \mathbf{u})} \quad (2)$$

We assume that the absolute value of each element of $\delta \mathbf{u}$ is smaller than that of $\mathbf{u} - u_i \hat{\mathbf{e}}_i$. Then, by ignoring $\delta \mathbf{u}$ in Eq. (2) and substituting the expression for ΔL in Eq. (2), we obtain

$$\Delta \lambda_2 \approx \frac{\sum_{j \in \mathcal{N}_i} u_j (u_i - u_j)}{1 - u_i^2}, \quad (3)$$

where \mathcal{N}_i indicates the neighborhood of node i .

In the perturbative strategy, we remove node i that maximizes $\Delta \lambda_2$ given by Eq. (3). Note that carrying out one step of the perturbative strategy requires solving the eigen equation just once. Therefore, the computation cost is $O(N^3)$, which is N times smaller than that for the optimal sequential strategy. In the following numerical simulations, the networks are connected during sequential node removal for all the networks and strategies.

III. RESULTS

In this section, we apply the node-removal strategies introduced in Sec. II to various model and real networks.

A. Model networks

First, we apply different strategies to the following types of model networks.

- Erdős-Rényi (ER) random graph with mean degree $\langle k \rangle = p(N - 1)$, where p is the probability that a link exists between a pair of nodes.

- Watts-Strogatz (WS) model [27], where each node is connected to $\langle k \rangle / 2$ closest nodes on each side along the ring and a fraction, 0.3, of links are rewired randomly.
- Barabási-Albert (BA) model [28], a representative growing scale-free network model. We start the growth of the network from the complete graph of m nodes and add a node with m links one-by-one according to the preferential attachment. We obtain $\langle k \rangle \approx 2m$, degree distribution $p(k) \propto k^{-3}$, and low clustering.
- Holme-Kim (HK) model [29], a growing scale-free network model. The algorithm of the HK model is similar to that of the BA model. The difference is that, when a node is added, the preferential attachment is used with a certain probability, which we set as 0.5. With the remaining probability (*i.e.*, 0.5), we use the so-called triad formulation rule to enhance clustering. We obtain $\langle k \rangle \approx 2m$, degree distribution $p(k) \propto k^{-3}$, and high clustering.
- Goh model [30], a nongrowing scale-free network model. We assign the weight $w_i = i^{-0.5}$ to each node i . Then, we select a pair of nodes with the probability proportional to w_i and connect them. We repeat this procedure until we obtain the desired mean degree $\langle k \rangle$. We obtain $p(k) \propto k^{-3}$.

For each network model, we assume two values of $\langle k \rangle$. For each case, we carry out sequential node removal according to different strategies. Because, in stepwise node removal, the optimal sequential strategy is usually an efficient way, we will mainly evaluate the effectiveness of the other strategies using the performance of the optimal sequential strategy as a baseline.

The numerical results obtained for the networks with $N = 250$ averaged over 10 trials are shown in Fig. 1. Figures 1(a)(1) and 1(a)(2) show the values of λ_2 after removing a fraction of nodes for two ER random graphs with different values of $\langle k \rangle$. The fraction of the removed nodes is denoted by f . For each strategy, λ_2 increases slightly in the early stages (*i.e.*, $0 < f < 0.05$). Then, λ_2 starts to decrease even for the optimal sequential and perturbative strategies, which are designed to maximize λ_2 . Surprisingly, in the network with larger $\langle k \rangle$ (Fig. 1(a)(2)), the optimal sequential strategy is not as efficient as the other strategies as f increases. This is possible because the optimal sequential strategy finds the stepwise best strategy and does not take into account the performance after multiple nodes are removed. The perturbative strategy remains more efficient or as efficient as the optimal sequential strategy when f is large.

For the WS model with different mean degrees (Fig. 1(b)(1) and 1(b)(2)), the optimal sequential and perturbative strategies outperform the heuristic degree-based and betweenness-based strategies. As in the case of the ER random graph, the perturbative strategy is as efficient as the optimal sequential strategy.

The performances of the perturbative strategies are also good among the competitive strategies for different scale-free network models (Fig. 1(c)(1), 1(c)(2), 1(d)(1), and 1(d)(2)). In Goh model (Fig. 1(e)(1) and 1(e)(2)), though it is not better than the degree-based strategy, the perturbative strategy is better than the optimal sequential strategy except for in the early stage (*i.e.* $0 < f < 0.3$) in the Goh model with the smaller degree (Fig. 1(e)(1)). Note that for the three scale-free network models, λ_2 continues to increase even until half the nodes are removed.

Changes in $\langle k \rangle$ and the standard deviation of the degree with node removal according to the perturbative strategy are shown in Fig. 1(a)(3), 1(a)(4), 1(b)(3), 1(b)(4), 1(c)(3), 1(c)(4), 1(d)(3), 1(d)(4), 1(e)(3), and 1(e)(4). The direction of changes in $\langle k \rangle$ and that of the standard deviation of the degree depend on the network model. For example, in the Goh model, nodes with small degree are preferentially removed in general, especially for small f (Fig. 1(e)(3)). However, the removed nodes are not generally those with the smallest degrees; the degree-based strategy performs relatively poorly (Fig. 1(b)(1), 1(b)(2), 1(c)(1), 1(c)(2), 1(d)(1), 1(d)(2), 1(e)(1), and 1(e)(2)). In contrast, in the ER, WS, BA, and HK models, the perturbative strategy removes nodes with appropriately large degree (Fig. 1(a)(3), 1(b)(3), 1(c)(3), and 1(d)(3)). Similarly, the perturbative strategy increases λ_2 by increasing the heterogeneity of degree in the WS model (Fig. 1(b)(4)) and by decreasing the same heterogeneity in the other four network models (Fig. 1(a)(4), 1(c)(4), 1(d)(4), and 1(e)(4)). These show that the perturbative strategy adapts itself for each network.

Next, we compare the efficiency of different strategies on larger networks ($N = 2000$). We exclude the optimal sequential strategy because the large N hinders its implementation. In this set of numerical simulations, we are mainly concerned with the performance of the perturbative strategy. The numerical results obtained on the basis of 5 realizations of each network are shown in Fig. 2. These results are qualitatively the same as those obtained for the smaller networks shown in Fig. 1. The perturbative strategy enhances λ_2 more efficiently than the other heuristic strategies except in ER models. In addition, the behavior of the perturbative strategy cannot be simply captured by the changes in $\langle k \rangle$ or the standard deviation of the degree, which is again qualitatively the same as the results shown in Fig. 1.

B. Real networks

We apply the proposed strategies to the largest connected component of the following real networks: the *C. elegans* neural network [31, 32], *E. coli* metabolic network [33], e-mail social network [34], and macaque cortical network [35]. We ignore the direction of links in the *C. elegans* neural network and the macaque cortical network, both of which are originally directed networks. In the *C. elegans* neural network, two neurons are regarded to be connected when they are connected by at least one chemical synapse or gap junction.

The efficiency of different strategies on these real networks is shown in Fig. 3. The perturbative strategy enhances λ_2 more efficiently in all the tested real networks than the degree-based and betweenness-based strategies. Except in the case of the *E. coli* metabolic network, which is too large for the optimal sequential strategy, the results for the optimal sequential strategy are shown as well (Fig. 3(a), 3(c), and 3(d)). The perturbative strategy performs roughly as well as the optimal sequential strategy in these networks.

C. Comparison to the rewiring strategy

One can alternatively enhance λ_2 by rewiring links [8, 14]. In the rewiring strategy, we sequentially rewire links to increase λ_2 . In each step, we examine the increase in λ_2 for all the possible patterns of single-link rewiring and adopt the one that increases λ_2 by the largest amount. To compare the performance of the node removal and the rewiring, we carry out numerical simulations using the ER and BA models with $N = 50$ and $\langle k \rangle = 4$. We simulate the rewiring process just once for each network because the rewiring strategy is computationally costly.

The change in λ_2 relative to the initial value during the rewiring process is shown in Fig. 4(a). λ_2 is enhanced up to about 1.7 fold for both networks. The corresponding results for the sequential node removal according to the perturbative strategy are shown in Fig. 4(b). Roughly speaking, the performance of the perturbative strategy is comparable to that of the rewiring strategy. The perturbative strategy is superior to the rewiring strategy for the ER model and vice versa for the BA model. Because the rewiring strategy is computationally costly and may be too demanding to be implemented in some real applications, the node removal according to the perturbative strategy seems to be a feasible choice for enhancing λ_2 .

D. Accuracy of the perturbative strategy

When deriving the perturbative strategy, we crucially assumed that $\delta\mathbf{u}$ is negligible as compared to $\mathbf{u} - u_i\hat{\mathbf{e}}_i$. We justify this assumption as follows. A node that is removed according to the perturbative strategy tends to have large $\Delta\lambda_2$ and a small degree. If the removed node has a small degree, the number of the nonzero entries of the corresponding ΔL is relatively small. Therefore, a relatively small number of the entries of \mathbf{u} would be directly affected by the node removal, and we would obtain a small $\delta\mathbf{u}$.

To probe the validity of this assumption and quantify the error in estimating $\Delta\lambda_2$, we measure two kinds of relative estimation error during the course of sequential node removal according to the perturbative strategy. The first quantity is the average of $|(\delta\mathbf{u})_j/(\mathbf{u} - u_i\hat{\mathbf{e}}_i)_j|$ over node j ($1 \leq j \leq N$, $j \neq i$), where i is the index of the removed node. The second quantity is the difference between $\Delta\lambda_2$ obtained from the perturbative strategy and the actual $\Delta\lambda_2$, which is normalized by the actual $\Delta\lambda_2$. We take averages of these quantities over 200 generated networks having $N = 250$.

For the five network models, $|(\delta\mathbf{u})_j/(\mathbf{u} - u_i\hat{\mathbf{e}}_i)_j|$ for $\langle k \rangle = 10$ and $\langle k \rangle = 40$ is shown in Fig. 5(a) and 5(b), respectively. The magnitude of $\delta\mathbf{u}$ relative to that of $\mathbf{u} - u_i\hat{\mathbf{e}}_i$ is sufficiently small. The relative estimation error in $\Delta\lambda_2$ for the removed nodes is shown for $\langle k \rangle = 10$ and $\langle k \rangle = 40$ in Fig. 5(c) and 5(d), respectively. As expected, the relative estimation error in $\Delta\lambda_2$ is generally small. We conclude that, up to our numerical efforts, the perturbative strategy does not suffer from a crucially large error.

IV. CONCLUSIONS

We explored efficient strategies to sequentially remove nodes of networks in order to increase or maintain a large value of the spectral gap (*i.e.*, second smallest eigenvalue of the Laplacian matrix) of the undirected and unweighted network. We introduced a perturbative strategy among others. For a variety of networks, this strategy generally performed well as compared to heuristic strategies in which we sequentially remove the nodes with the smallest degree or the smallest betweenness centrality. In most of our numerical results, the spectral gap increased until the removal of a fairly large fraction of nodes ($\approx 50\%$). Occasionally, the perturbative strategy is even more efficient than the optimal sequential strategy, despite its

decreased computational cost. Although we focused on unweighted networks, the extension of the perturbative strategy to the case of weighted networks is straightforward.

In chaotic dynamical systems on networks, synchronization is often facilitated by a small value of $R = \lambda_N/\lambda_2$, where λ_2 and λ_N are the second smallest eigenvalue and the largest eigenvalue of the Laplacian matrix, respectively. Dynamics whose synchronizability is determined by R belongs to the class III [2, 9] (also termed type I [4]). In contrast, we have been concerned with the synchronization of the class II [2, 9] (also termed type II [4]) dynamics in which synchronization is facilitated in networks with large λ_2 . To address class III or type I synchronizability, we developed the perturbative strategy for minimizing R upon the removal of nodes and assessed its efficiency on some model networks. However, the results were generally poor (results not shown). The perturbative strategy failed mainly because it does not accurately estimate the change in λ_N . The applicability of our results is limited to class II or type II dynamics.

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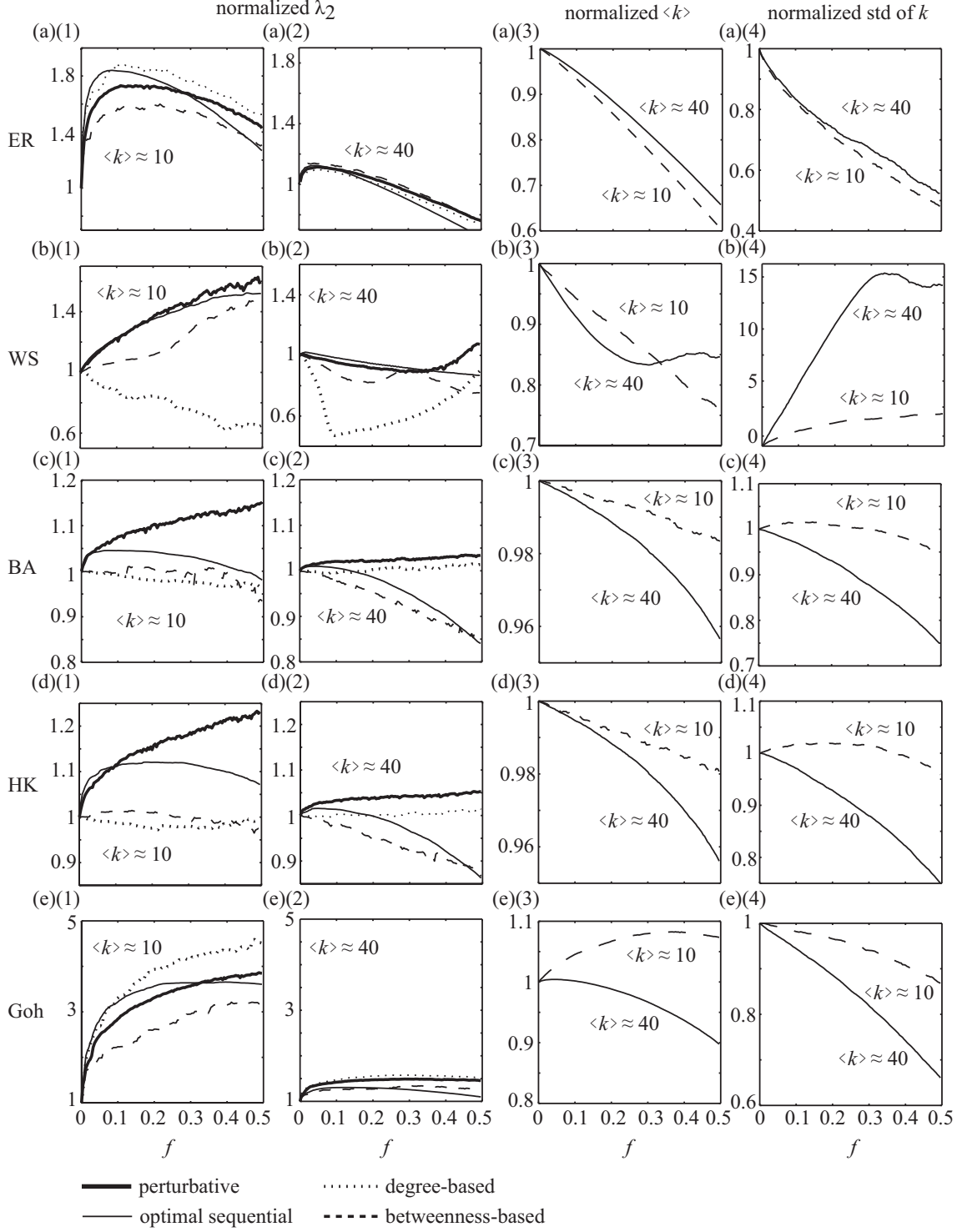


FIG. 1: Numerical results for model networks with $N = 250$ nodes. We set $\langle k \rangle = 10$ and $\langle k \rangle = 40$ for each network. (a) ER random graph, (b) WS model, (c) BA model, (d) HK model, and (e) Goh model. (a)(1), (a)(2), (b)(1), (b)(2), (c)(1), (c)(2), (d)(1), (d)(2), (e)(1), and (e)(2) show the change in λ_2 induced by each strategy. The mean degrees are shown in the panels. (a)(3), (b)(3), (c)(3), (d)(3), and (e)(3) show the change in the mean degree with node removal. (a)(4), (b)(4), (c)(4), (d)(4), and (e)(4) show the change in the standard deviation of the degree with node removal.

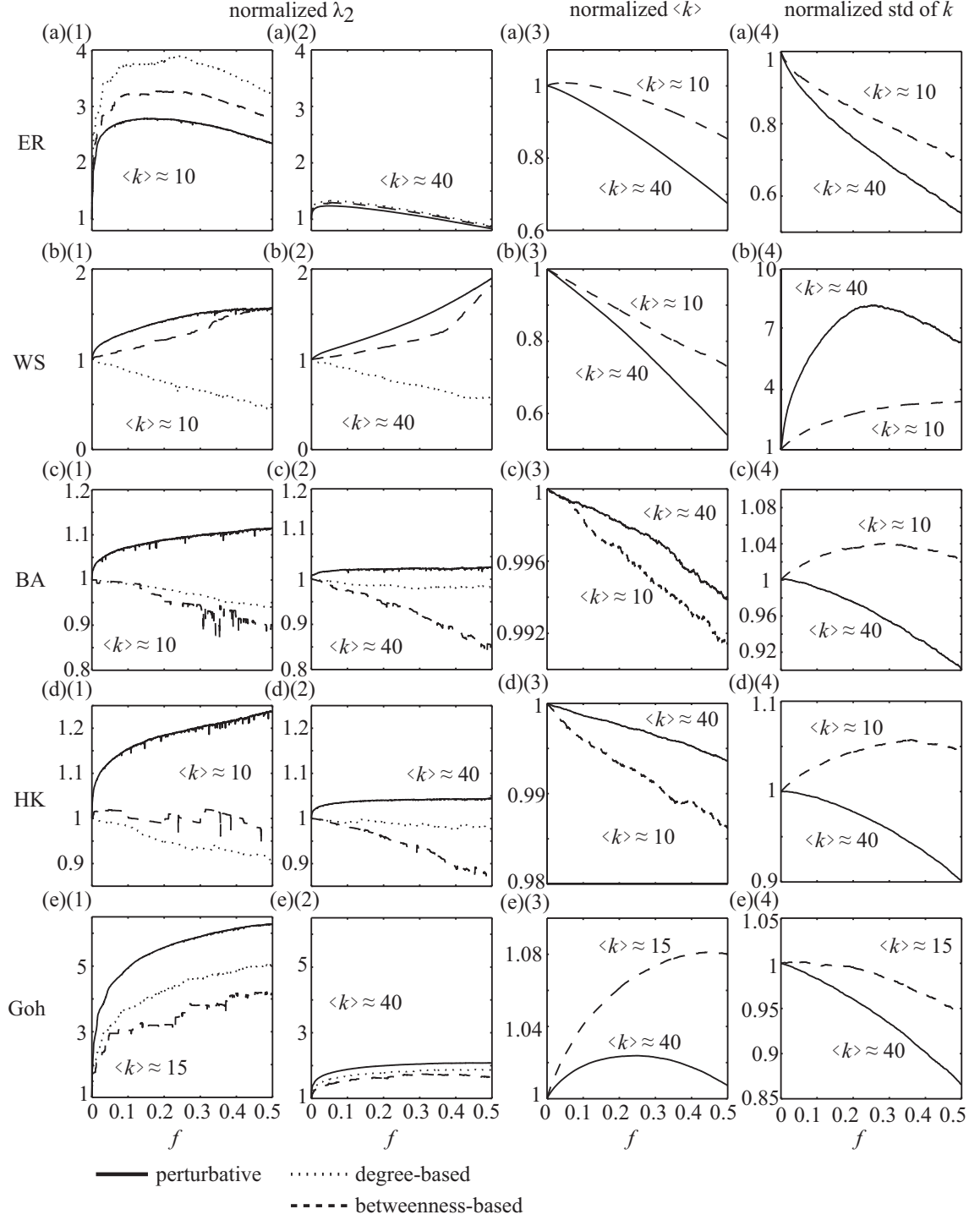


FIG. 2: Numerical results for (a) ER model, (b) WS model, (c) BA model, (d) HK model, and (e) Goh model with $N = 2000$. We set $\langle k \rangle = 10$ and $\langle k \rangle = 40$ for each network model with one exception. We use $\langle k \rangle = 15$ instead of $\langle k \rangle = 10$ for the Goh model because the Goh model with $N = 2000$, $\langle k \rangle = 10$, and $w_i = i^{-0.5}$ ($1 \leq i \leq N$) rarely yields a connected network.

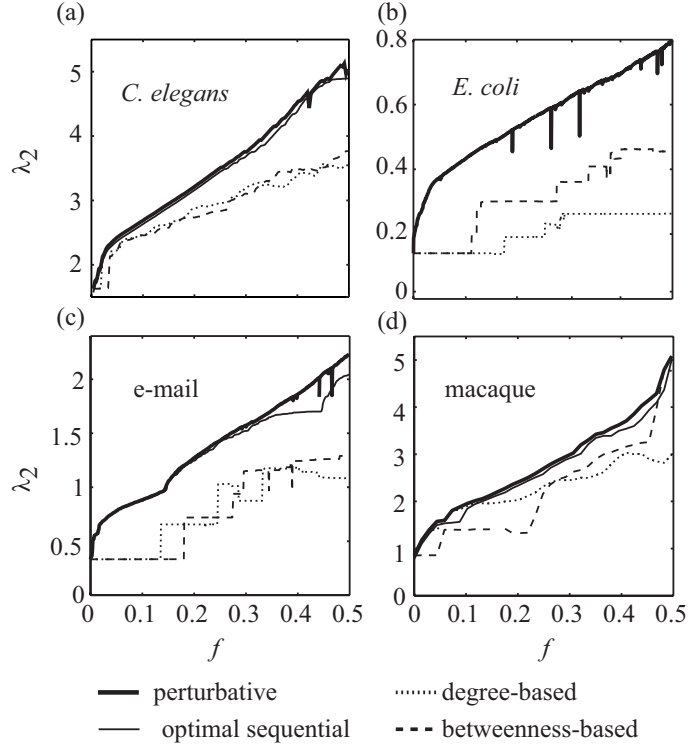


FIG. 3: Numerical results for real networks. (a) *C. elegans* neural network with $N = 279$ and $\langle k \rangle = 16.4$. (b) *E. coli* metabolic network with $N = 2268$ and $\langle k \rangle = 4.96$. (c) E-mail social network with $N = 1133$ and $\langle k \rangle = 9.62$. (d) Macaque cortical network with $N = 71$ and $\langle k \rangle = 12.3$.

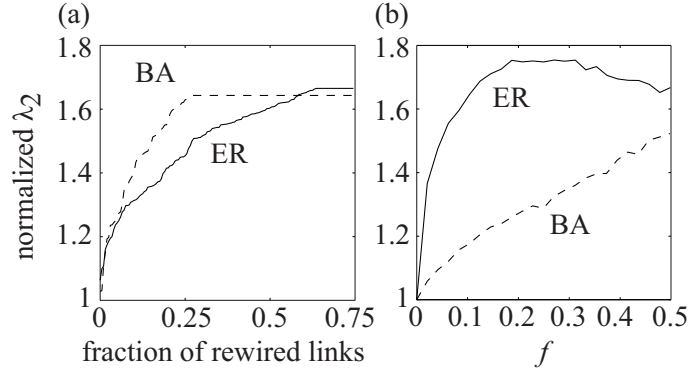


FIG. 4: Numerical results for the ER and BA models with $N = 50$. (a) Results for link rewiring. The normalized λ_2 is plotted against the number of rewired links. (b) Results for node removal. The normalized λ_2 averaged over 10 realizations is plotted against the number of removed nodes. We set $\langle k \rangle = 4$ in both networks.

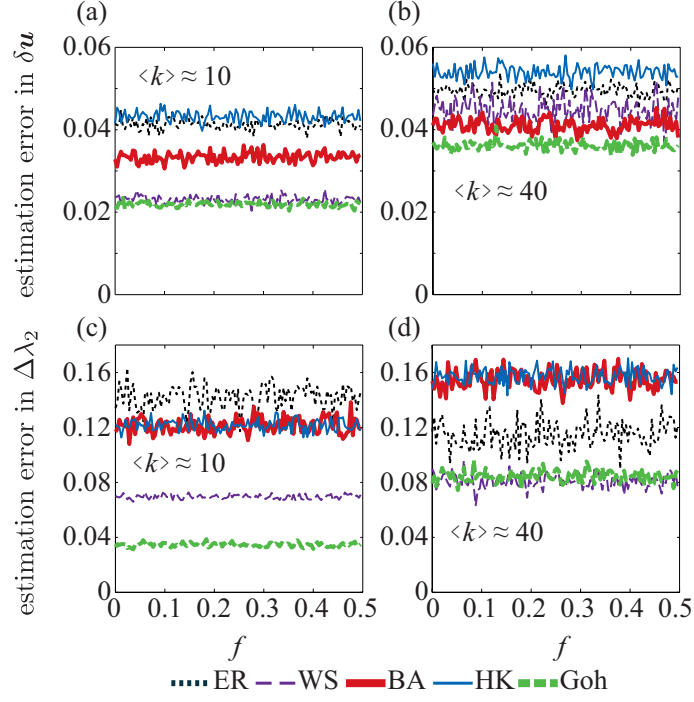


FIG. 5: (Color online) Relative estimation error in (a, b) $\delta \mathbf{u}$ and (c, d) $\Delta \lambda_2$. See Sec. IIID for the definitions of the relative estimation error. We set (a, c) $\langle k \rangle = 10$ and (b, d) $\langle k \rangle = 40$. We use $\langle k \rangle = 15$ instead of $\langle k \rangle = 10$ for the Goh model because the Goh model with $N = 250$, $\langle k \rangle = 10$, and $w_i = i^{-0.5}$ ($1 \leq i \leq N$) rarely yields a connected network.